

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
 Data File : BM028497.D
 Acq On : 21 Jan 2021 20:31
 Operator : CG/JU
 Sample : M1179-08
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 HS-TP4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028497.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	310	319	326	rBV	9979	15528	1.57%	0.242%
2	5.540	393	400	410	rVB	401040	575251	58.06%	8.961%
3	6.669	588	592	596	rBV	10262	14650	1.48%	0.228%
4	7.175	671	678	688	rBV	390312	615922	62.16%	9.595%
5	8.016	815	821	827	rVB	112543	170351	17.19%	2.654%
6	9.192	1013	1021	1028	rBV	239058	388518	39.21%	6.052%
7	10.833	1292	1300	1307	rVB	142992	231209	23.33%	3.602%
8	13.280	1710	1716	1723	rBV	509775	751128	75.81%	11.701%
9	14.110	1853	1857	1863	rVB	9734	12775	1.29%	0.199%
10	14.657	1945	1950	1957	rVB	194663	281918	28.45%	4.392%
11	16.139	2196	2202	2213	rVB	423764	563153	56.84%	8.773%
12	17.386	2408	2414	2420	rBV	229084	314713	31.76%	4.903%
13	18.256	2557	2562	2568	rBV	45647	65994	6.66%	1.028%
14	18.333	2572	2575	2579	rVB	9708	11269	1.14%	0.176%
15	19.015	2686	2691	2695	rBV	55367	65744	6.64%	1.024%
16	19.103	2702	2706	2711	rBV2	15554	19712	1.99%	0.307%
17	19.409	2755	2758	2766	rVB5	8231	16074	1.62%	0.250%
18	19.521	2774	2777	2784	rBV3	19177	28182	2.84%	0.439%
19	19.645	2794	2798	2802	rBV	17337	20017	2.02%	0.312%
20	19.703	2805	2808	2812	rBV2	6900	10064	1.02%	0.157%
21	19.980	2849	2855	2860	rBV	831110	990836	100.00%	15.435%
22	20.168	2884	2887	2890	rBV	9207	11231	1.13%	0.175%
23	20.645	2964	2968	2972	rBV	30519	36529	3.69%	0.569%
24	20.709	2975	2979	2983	rBV	56304	66505	6.71%	1.036%
25	20.850	2998	3003	3007	rBV	158445	183065	18.48%	2.852%
26	20.892	3007	3010	3014	rVV	34608	40421	4.08%	0.630%
27	20.956	3018	3021	3024	rBV	13566	14508	1.46%	0.226%
28	21.215	3061	3065	3072	rBV	114474	141535	14.28%	2.205%
29	21.333	3082	3085	3088	rBV	20058	21566	2.18%	0.336%
30	21.515	3111	3116	3124	rBV	307223	380443	38.40%	5.926%
31	23.797	3499	3504	3512	rVB	191400	360574	36.39%	5.617%

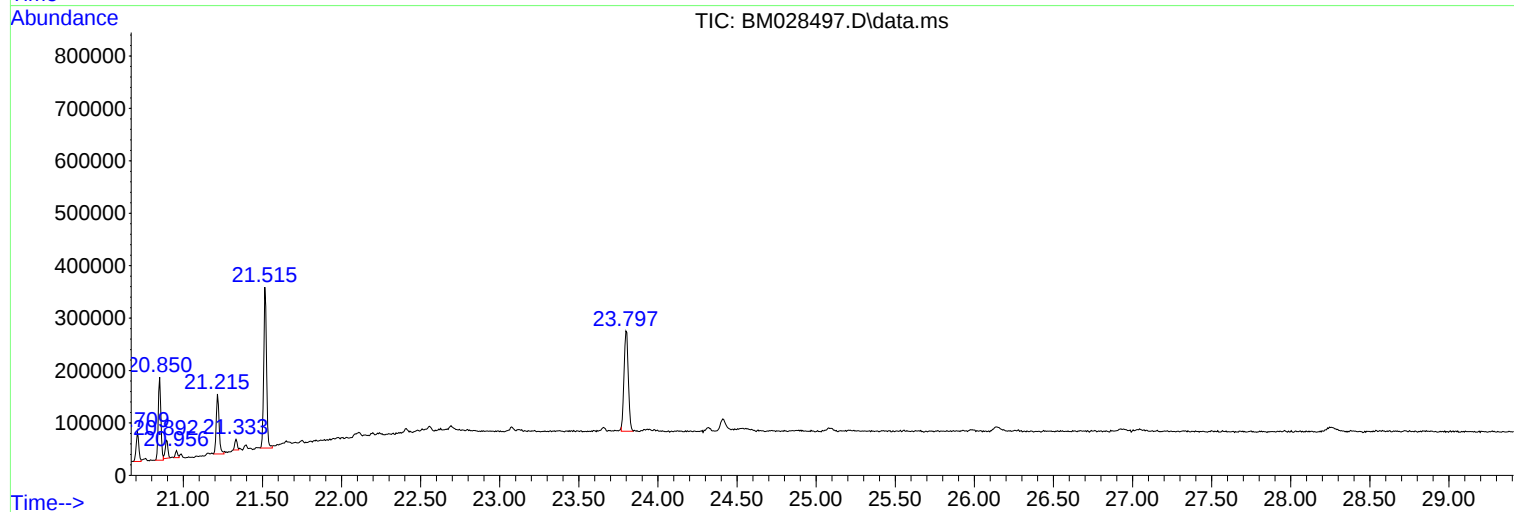
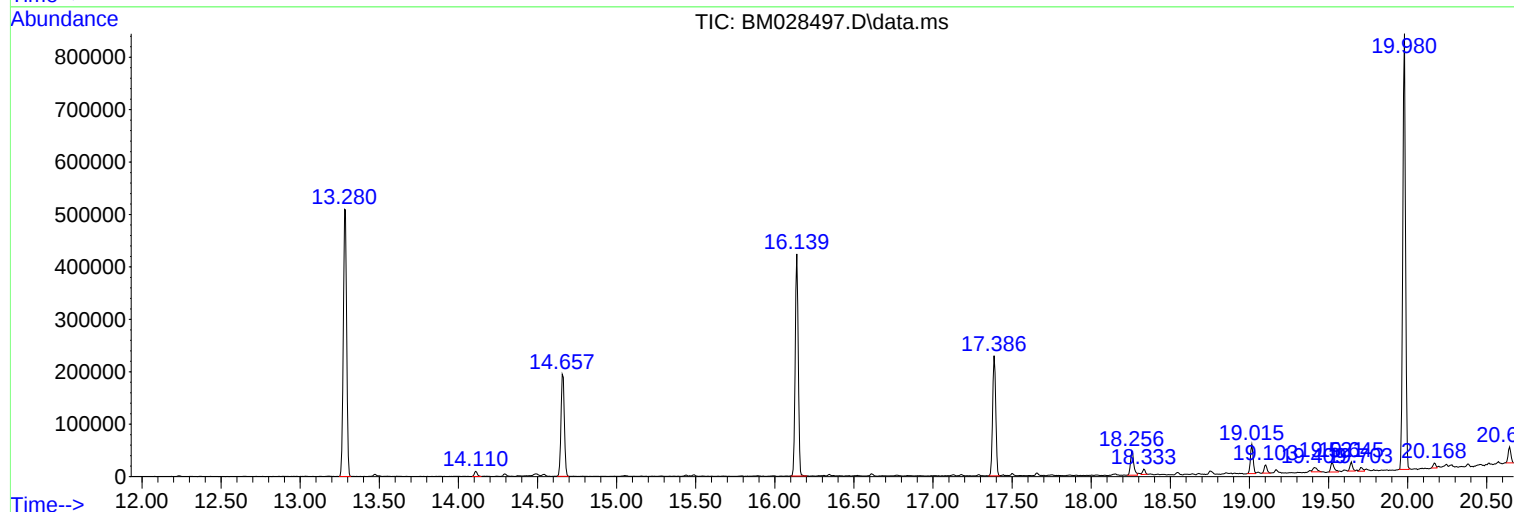
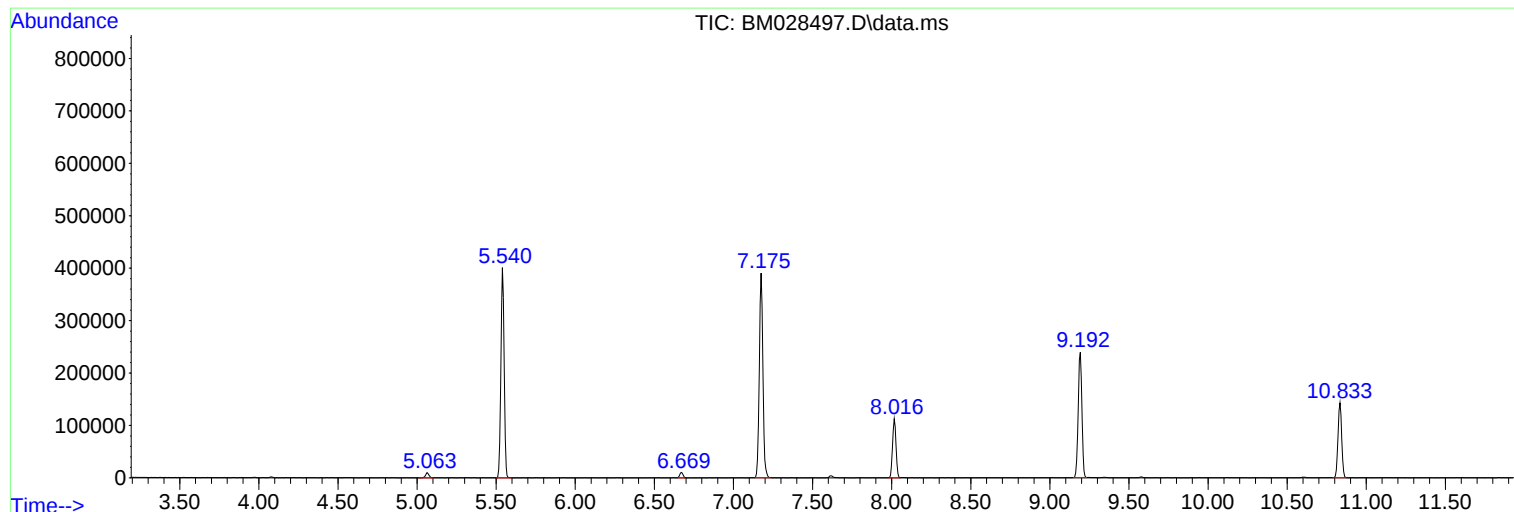
Sum of corrected areas: 6419385

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

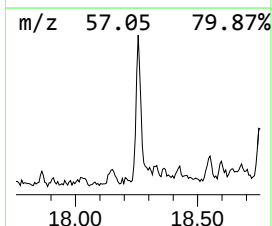
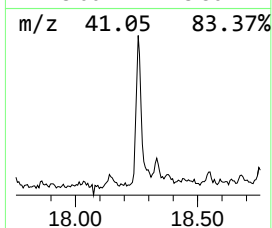
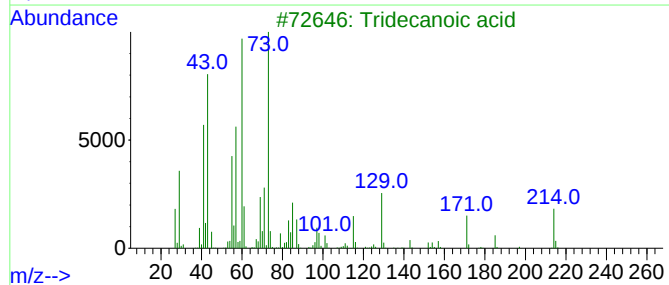
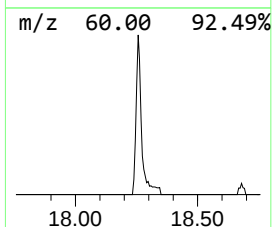
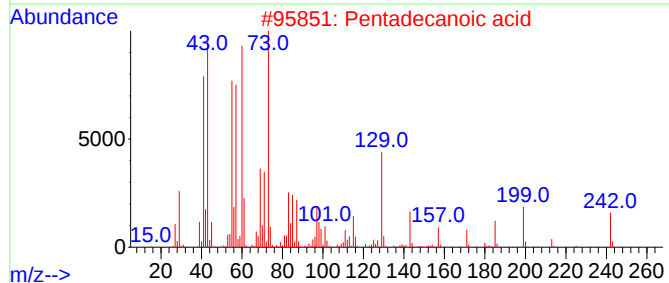
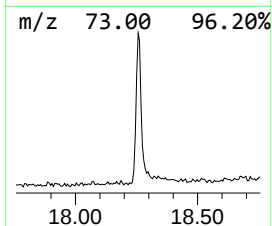
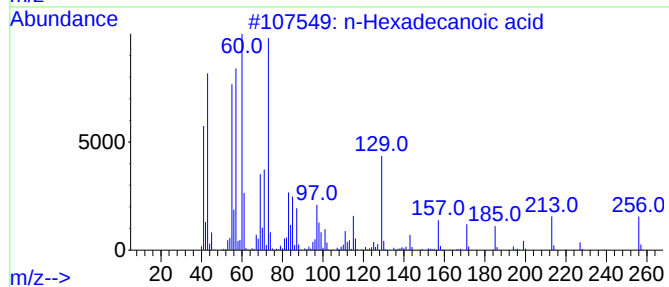
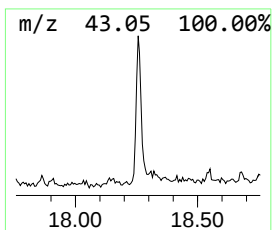
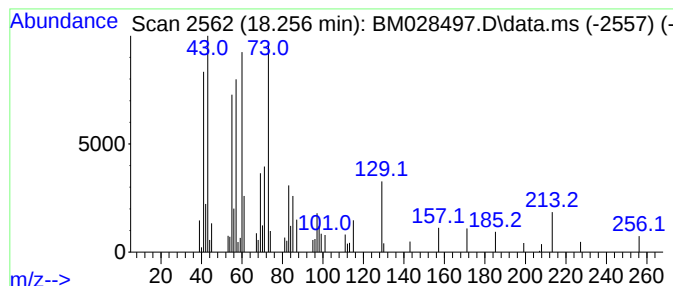
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.256	4.19 ng	65994	Phenanthrene-d10	17.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

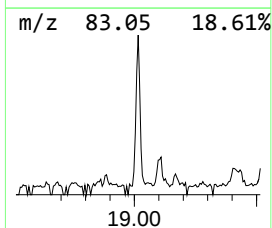
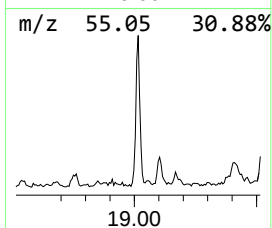
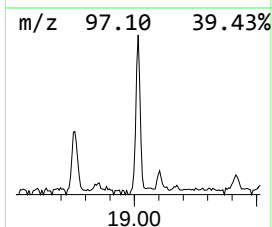
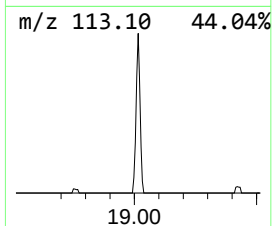
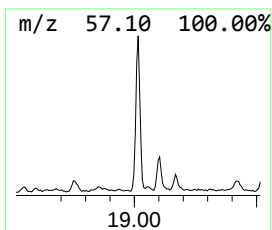
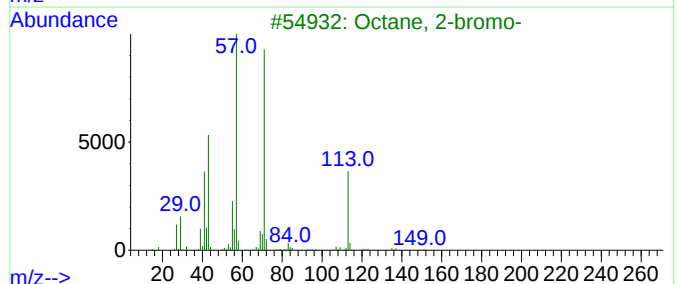
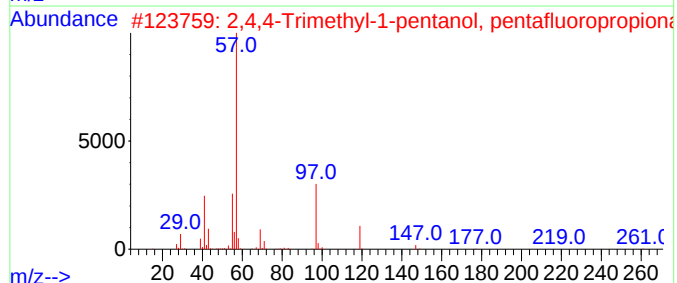
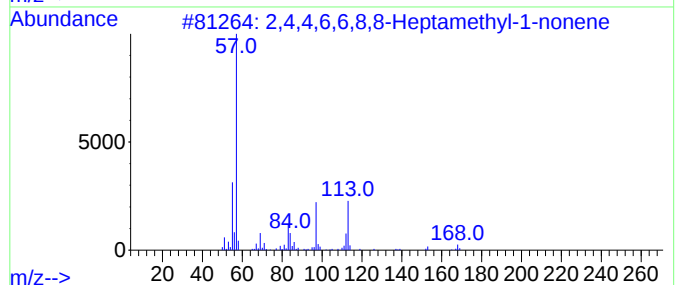
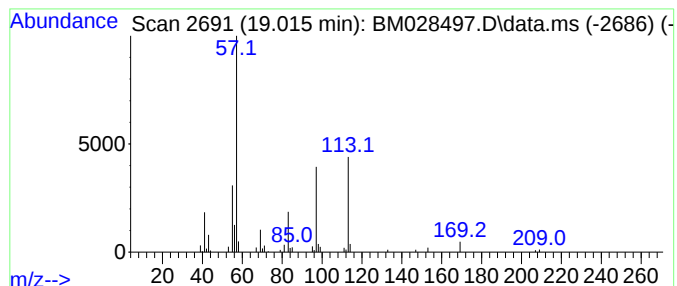
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown19.015 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	4.18 ng	65744	Phenanthrene-d10	17.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	47
2			2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	43
3			Octane, 2-bromo-	192	C8H17Br	000557-35-7	38
4			2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	38
5			2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

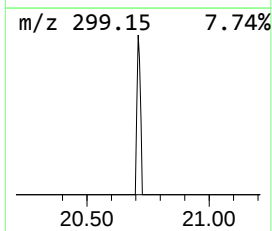
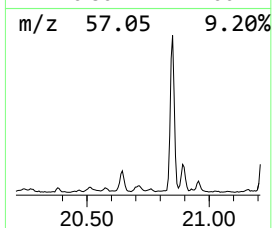
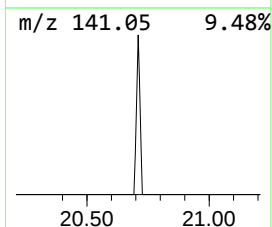
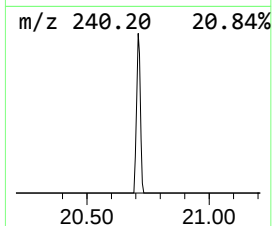
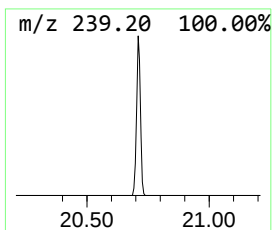
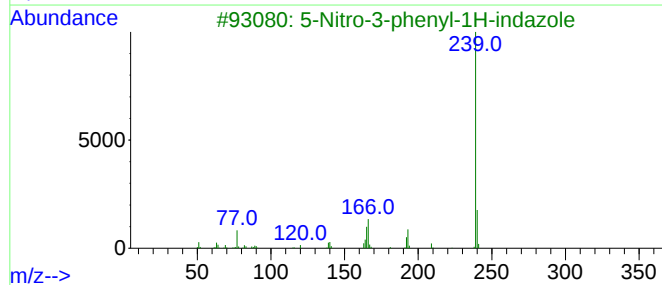
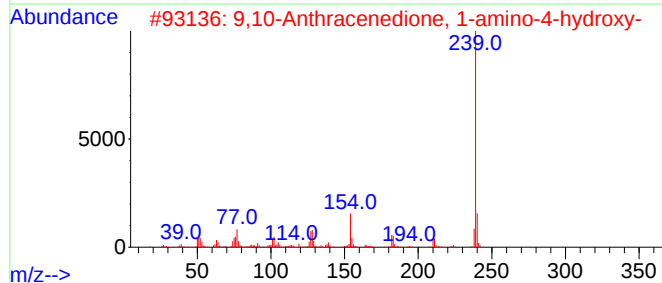
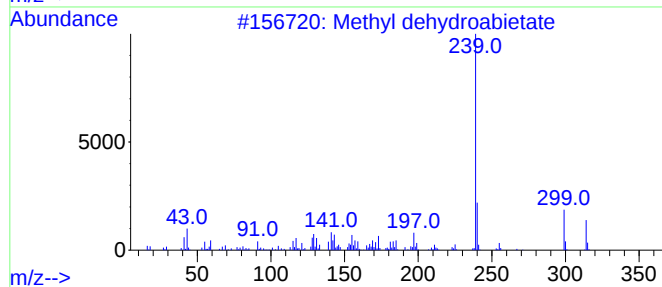
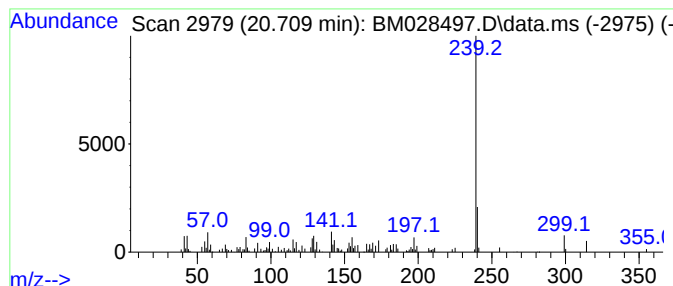
Instrument :
BNA_M
ClientSampleId :
HS-TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Methyl dehydroabietate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.709	3.50 ng	66505	Chrysene-d12	21.515	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl dehydroabietate	314	C21H30O2	001235-74-1	95
2	9,10-Anthracenedione, 1-amino-4-...	239	C14H9NO3	000116-85-8	64
3	5-Nitro-3-phenyl-1H-indazole	239	C13H9N3O2	293758-67-5	64
4	Terephthalic acid, di(2-methylph...	346	C22H18O4	1000323-60-7	59
5	2-(p-Acetylanilino)tropone	239	C15H13NO2	1000241-52-9	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

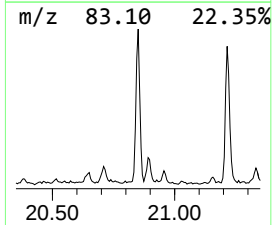
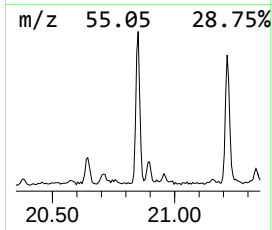
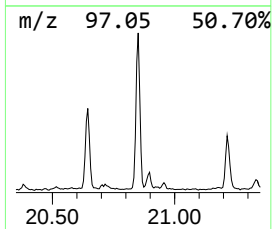
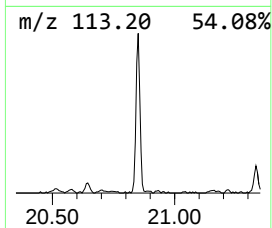
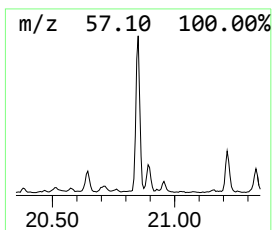
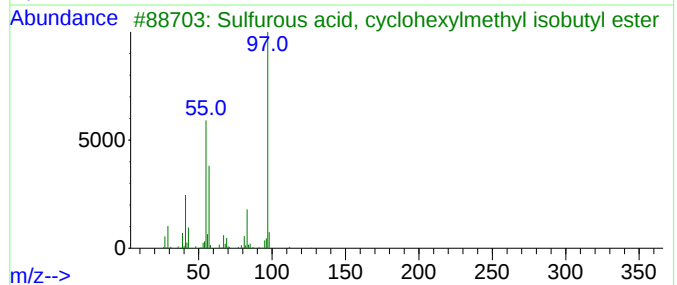
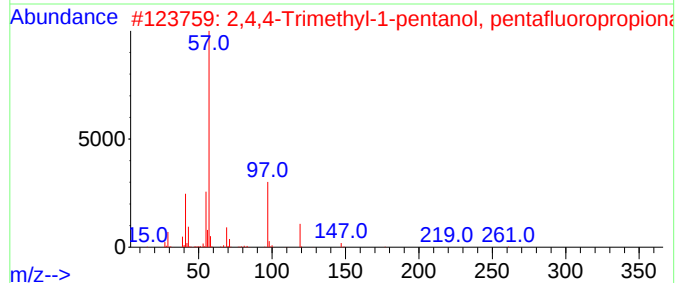
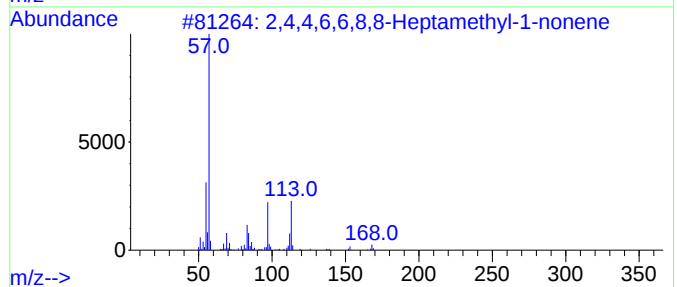
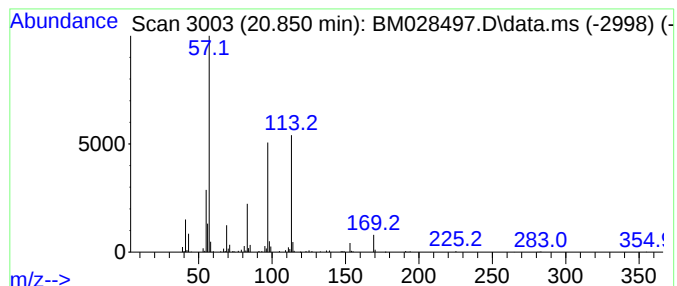
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.850	9.62 ng	183065	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	83		
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38		
3	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	37		
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	32		
5	Octane, 2-bromo-	192	C8H17Br	000557-35-7	32		



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

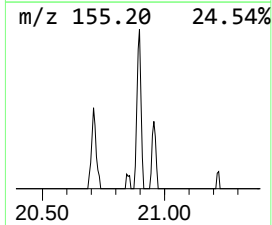
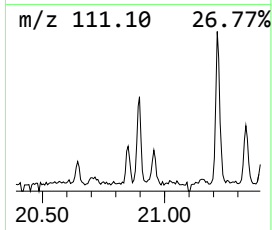
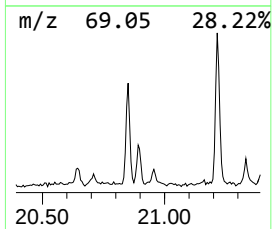
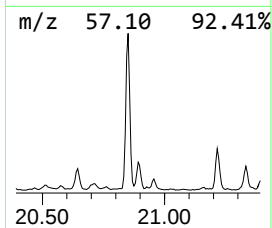
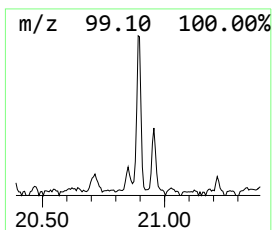
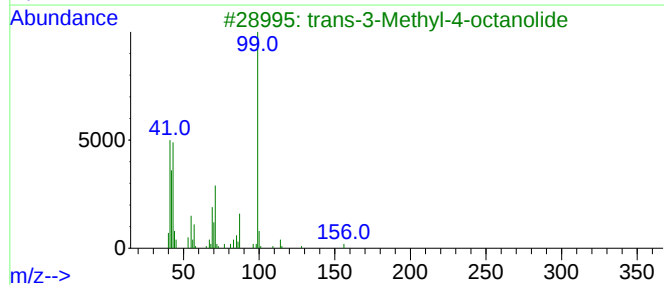
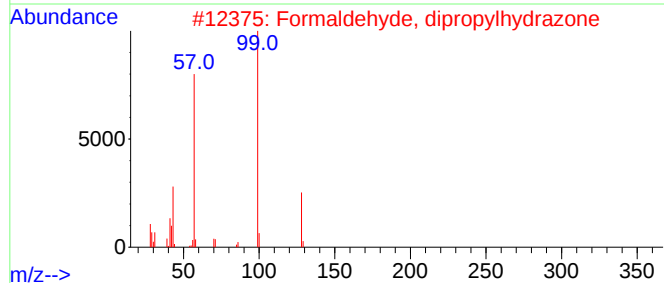
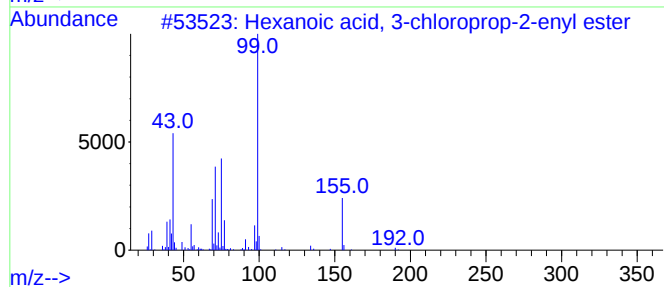
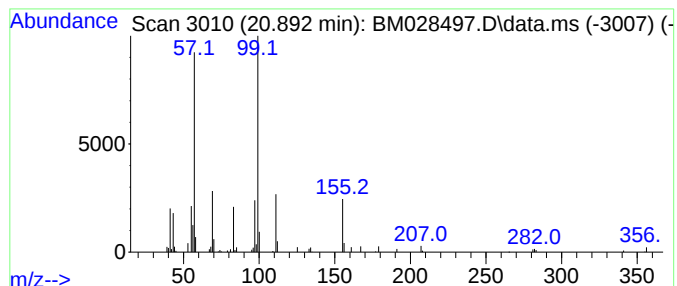
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown20.892 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.892	2.12 ng	40421	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3-chloroprop-2-en...	190	C9H15ClO2	1000299-36-1	47
2			Formaldehyde, dipropylhydrazone	128	C7H16N2	054253-56-4	37
3			trans-3-Methyl-4-octanolide	156	C9H16O2	039638-67-0	37
4			2-Piperidinone	99	C5H9NO	000675-20-7	35
5			1-Pyrrolidinocarbonylmethyl pipe...	197	C10H19N3O	039890-45-4	28



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

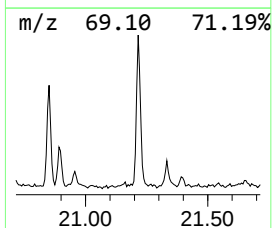
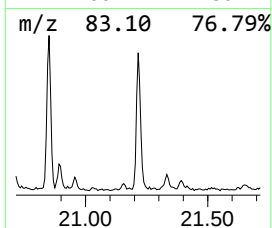
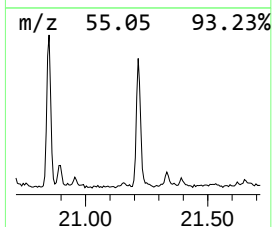
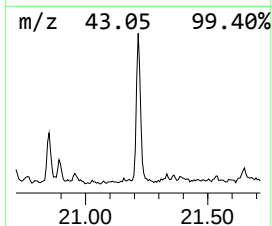
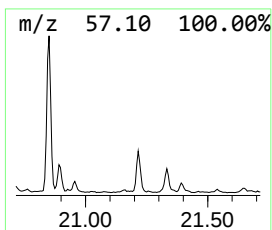
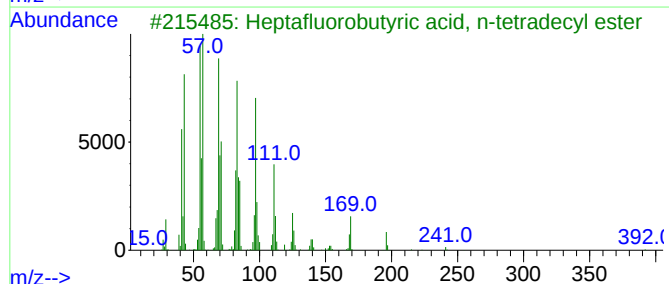
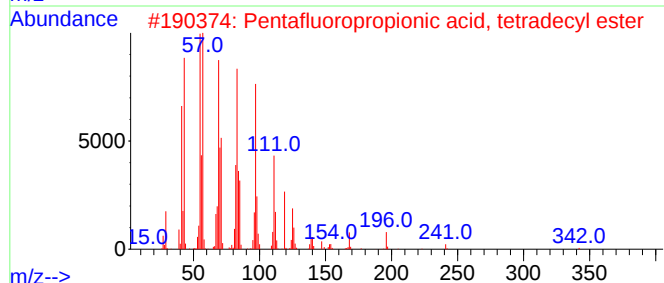
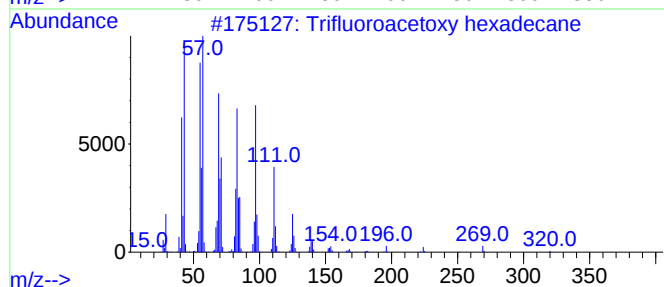
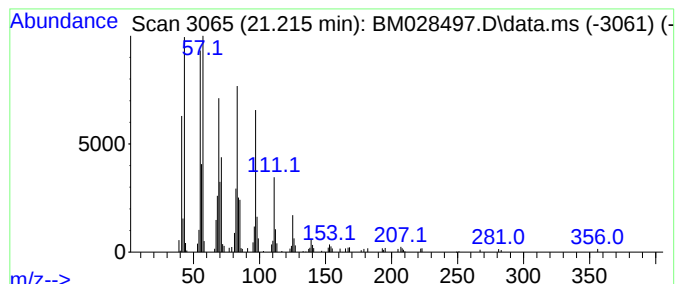
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.215	7.44 ng	141535	Chrysene-d12	21.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
3			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4			1-Heneicosanol	312	C21H44O	015594-90-8	93
5			n-Nonadecanol-1	284	C19H40O	001454-84-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012121\
Data File : BM028497.D
Acq On : 21 Jan 2021 20:31
Operator : CG/JU
Sample : M1179-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
HS-TP4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.256	4.2	ng	65994	4	17.386	314713	20.0
unknown19.015	19.015	4.2	ng	65744	4	17.386	314713	20.0
Methyl dehydroa...	20.709	3.5	ng	66505	5	21.515	380443	20.0
2,4,4,6,6,8,8-H...	20.850	9.6	ng	183065	5	21.515	380443	20.0
unknown20.892	20.892	2.1	ng	40421	5	21.515	380443	20.0
Trifluoroacetox...	21.215	7.4	ng	141535	5	21.515	380443	20.0